AD-A229 064

REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. AGENCY USE ONLY (Leave blank)	2. REPORT DATE	3. REPORT TYPE AND DATES COVERED
	2 Nov 1990	Final Report/1 Sep 84-31 Jul 90

4. TITLE AND SUBTITLE
RESONANCE ENERGIES AND WIDTHS FROM THE POLES OF THE MULTICHANNEL T MATRIX

5. FUNDING NUMBERS
61102F/2301/A4

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8. PERFORMING ORGANIZATION REPORT NUMBER
AFOSR-TR- 90 1145

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)
AFOSR/NP
Bolling AFB DC 20332-6448

10. SPONSORING/MONITORING AGENCY REPORT NUMBER
AFOSR-84-0379

11. SUPPLEMENTARY NOTES

12a. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution is unlimited.

12b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)
A multichannel iteration technique was developed to obtain accurate results for phase shifts from a "smooth" Schwinger K matrix. Applications were made to e + He^+ phase shifts in one, two, and three channel approximations. A second project was started to study excited states of helium using dimensional analysis. A moment method is being used to solve the two-electron Schrodinger equation generalized to an arbitrary number of dimensions.

14. SUBJECT TERMS

15. NUMBER OF PAGES
05

16. PRICE CODE

17. SECURITY CLASSIFICATION OF REPORT	18. SECURITY CLASSIFICATION OF THIS PAGE	19. SECURITY CLASSIFICATION OF ABSTRACT	20. LIMITATION OF ABSTRACT
UNCLASSIFIED	UNCLASSIFIED	UNCLASSIFIED	UL SAR

AFOSR-84-0379

Final Technical Report

1 Sep 84 - 31 Jul 90

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A method of determining Rydberg states and resonance parameters based on a "smooth" K matrix has been extended to multichannel cases. An energy independent projection operator formalism to ensure orthogonality has been developed and a multichannel iteration procedure has now been successfully formulated. We have obtained accurate results for the ^1P, ^3P and ^3S Rydberg states of helium and for phase shifts using two channels at positive energies. We are presently working on the implementation of an improved multichannel iteration formalism which we hope will converge the three channel results to values which are independent of the initial basis set.

During the last year of the grant we began an investigation of excited states of helium using dimensional perturbation theory. We have successfully obtained energies for some singly-excited states of helium and have also completed a study of some $^{1,3}P^e$ states using inter-dimensional degeneracies.

Final Technical Report

This final report summarizes the research performed under Grant No. AFOSR-84-0379 from, September 1987, the date of the most recent Final Technical Report, to July 1990 when this grant terminated. The goal of this proposal, "Resonance Energies and Widths from the Poles of the Multichannel T Matrix" was to determine Rydberg and resonance poles using a "smooth" K matrix. Previous calculations had successfully determined Rydberg states of some alkali atoms and beryllium as well as resonance states for beryllium and H^- by searching for the poles of the complex T matrix. The present technique avoids both the use of complex arithmetic and individual searches for each pole by formulating a "smooth" K matrix which is real and free of poles. This is done by using alternative boundary conditions to define a "smooth" Green's function which is then used to determine the K matrix. Since this K matrix has no poles at bound-state energies, a smooth quantum defect curve can be defined at all negative energies. Determining bound state energies from this curve was found to be much more efficient than performing individual searches in a single-channel study of the Rydberg states of the lithium isoelectronic sequence. At positive energies a phase shift curve can be used to extract resonance parameters using a Breit-Wigner fit. The major goal of the present grant was to extend this new K matrix method to multichannel Rydberg and resonance studies. This required the development of a multichannel "smooth" Green's function and K matrix. Implementing this formalism also required the development of a projection operator formalism to ensure that the Rydberg electron is orthogonal to the core. A further goal was to develop a multichannel iteration technique to converge results after an initial basis set is chosen.

In summary, the Research Objectives as described above are:

1. Extension of the K matrix method to multichannel Rydberg and resonance states
2. Development of a numerical multichannel "smooth" Green's function
3. Development of a projection operation formalism to enforce orthogonality
4. Development of a multichannel iteration technique
5. Application to H^- and He.

We first focused on the Rydberg states of helium using two channels. We were able to obtain very good agreeement with experimental energies for the ^1P, ^3P and ^3S states of helium. The basis set consisted of solutions from single-channel calculations, four basis vectors in the first channel and a single basis vector in the second channel. Iteration was not necessary to obtain satisfactory results. An energy-independent projection operator formalism was successfully implemented and the effect of the closed channels was included by using a reduced K matrix formalism. This work was presented at the 19th annual meeting of the Division of Atomic, Molecular and Optical Physics in Baltimore in April 1988 and is presently being prepared for publication in Phys. Rev A.

Publications:

T. L. Goforth and D. K. Watson, "Multichannel Quantum Defect Calculations Using a Smooth Reaction Matrix", to be submitted, Phys. Rev. A.

This method was then extended to positive energies. Accurate results for phase shifts using one or two channels were easily obtained. For three channels we found that iteration in all channels became very important for accurate results. We believe we now have an improved multichannel iteration formalism which will enable us to obtain phase shifts and resonance parameters that are independent of the initial basis set.

This work was presented at the Sixteenth International Conference on the Physics of Electronic and Atomic Collisions in New York City in July 1989.

A second project was started in March of 1989 when a postdoctoral fellow, David Goodson, joined the group. We are investigating a new way of studying atomic phenomena called dimensional scaling or dimensional perturbation theory. The particular goal of this project is to study resonance states of helium using these techniques. Dimensional analysis obtains information about physical systems by generalizing the Schrodinger equation to an arbitrary number of dimensions. A moment method is being used to solve this generalized Schrodinger equation for some excited states of helium. We have chosen to formulate the problem using normal coordinates corresponding to the normal modes of vibration to take advantage of the pseudomolecular nature of the electron-nucleus-electron system. We are hopeful that this approach will provide insight into the geometry of resonance states of helium as well as provide meaningful quantum numbers for these strongly correlated states which are not well described by independent particle models. We presently have successfully obtained energies for some singly-excited states of helium and are analyzing the behavior of their asymptotic energy series. We have also completed a study of some interdimensional degeneracies between D=3 and D=5 which allows very accurate $^{1,3}P^e$ states for D=3 to be determined from S states in 5 dimensions. A description of this work has been prepared for publication in Phys. Rev. A.

Publications:

D. Goodson, D. K. Watson, J. G. Loeser and D. R. Herschbach, "Energies of Doubly-Excited Two-Electron Atoms from Interdimensional Degeneracies", to be submitted, Phys. Rev. A.

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